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ATOMS, MOLECULES AND STOCHIOMETRY

1. Relative masses atoms and molecules

1.1 Relative atomic mass, A_r

- The relative atomic mass (A_r) of an element is the mass of an atom relative to one twelth of the mass of an atom of carbon-12
- The unified atomic mass is defined as one-twelfth of the mass of a carbon-12 isotope (1 *u* = 1.66 x 10^{-27} kg)
- The A_r has no units as it is a ratio and the units cancel each other out

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$$\text{Relative atomic mass of an element } X = \frac{average\ mass\ of\ one\ atom\ of\ X}{1/12\ of\ the\ mass\ of\ one\ carbon{-}12\ atom}$$

1.2 Relative isotopic mass

- Atoms of the same element with a different number of neutrons are called isotopes
- Relative isotopic mass - the mass of an atom of an isotope relative to one twelfth of the mass of an atom of carbon-12
  - To calculate the average atomic mass of an element the percentage abundance is taken into account
  - Multiply the atomic mass of isotope by the percentage abundance for each isotope and add them all together
  - Divide by 100 to get average relative atomic mass
  - This is known as the weighted average of the masses of the isotopes

$$\text{RELATIVE ATOMIC MASS} = \frac{\sum(\text{ISOTOPE ABUNDANCE x ISOTOPE MASS NUMBER})}{100}$$

(WHERE ∑ = SUM OF)

1.3 Relative molecular mass, M_r

- The relative molecular mass (M_r) is the mass of a molecule relative to one twelfth of the mass of an atom of carbon-12
- The M_r has no units

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$$M_r = \frac{weighted\ average\ mass\ of\ molecules\ in\ a\ given\ sample\ of\ a\ molecular\ compound}{unified\ atomic\ mass\ unit}$$

- The M_r can be found by adding up the relative atomic masses of all atoms present in one molecule (the formula unit is used to calculate – silicon dioxide (SiO_2)

Substance	Atoms Present	M_r
Hydrogen (H_2)	2 x H	(2 x 1) = 2
Water (H_2O)	(2 x H) + (1 x O)	(2 x 1) + 16 = 18

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1.4 Relative formula mass, M_r

- The relative formula mass (M_r) is used for compounds containing ions
- It has the same units and is calculated in the same way as the relative molecular mass

Substance	Atoms Present	M_r (Relative Molecular Mass)
Potassium Carbonate K_2CO_3	$(2 \times K) + (1 \times C) + (3 \times O)$	$(2 \times 39) + 12 + (3 \times 16) = 138$
Calcium Hydroxide $Ca(OH)_2$	$(1 \times Ca) + (2 \times O) + (2 \times H)$	$40 + (2 \times 16) + (2 \times 1) = 74$
Ammonium Sulfate $(NH_4)_2SO_4$	$(2 \times N) + (8 \times H) + (1 \times S) + (4 \times O)$	$(2 \times 14) + (8 \times 1) + 32 + (4 \times 16) = 132$

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2. The mole and the Avogadro constant

- The Avogadro constant (N_A or L) is the number of particles equivalent to the relative atomic mass or molecular mass of a substance
  - The Avogadro constant applies to atoms, molecules, ions and electrons
  - The value of N_A is 6.02×10^{23} g mol^{-1}

- The mass of a substance with this number of particles is called a mole (mol)
  - The mass of a substance containing the same number of fundamental units as there are atoms in exactly 12.00 g of ^{12}C

1 mole of	Number of Atoms	Number of Molecules	Relative Mass (g)
Na	6.02×10^{23}	–	22.99
H_2	1.204×10^{24}	6.02×10^{23}	2.01
NaCl	1.204×10^{24}	6.02×10^{23}	58.44

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3. Formulae

3.1 Charges of ionic compounds

		+H						18
1	2		13	14	15	16	17	
Li^+	Be^{2+}					O^{2-}	F^-	
Na^+	Mg^{2+}		Al^{3+}				Cl^-	
K^+	Ca^{2+}	Transition Elements	Ga^{3+}			S^{2-}		
Rb^+	Sr^{2+}						Br^-	

Ion	Formula and Charge
Silver (I)	Ag^+
Ammonium	NH_4^+
Zinc (II)	Zn^{2+}
Hydroxide	OH^-
Nitrate	NO_3^-
Sulfate	SO_4^{2-}
Carbonate	CO_3^{2-}
Hydrogen ca	HCO_3^-
Phosphate	PO_4^{3-}

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While writing equations of a reaction:

Construct equations (which should be balanced), including ionic equations (which should not include spectator ions)

Use appropriate state symbols in equations

3.2 Empirical and molecular formula

Empirical formula

- The empirical formula is the simplest whole number ratio of the elements present in one molecule or formula unit of the compound
- It is calculated from knowledge of the ratio of masses of each element in the compound
- Can be found from the mass or the percentage composition of each element in the compound

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Determine the empirical formula of a compound that contains 10 g of hydrogen and 80 g of oxygen.

	Hydrogen (H)	Oxygen (O)
Mass of each element (g)	10 g	80 g
Divide by atomic mass	10 / 1.0 = 10 mol	80 / 16 = 5.0 mol
Divide by lowest figure to get ratio	10 / 5.0 = 2.0	5.0 / 5.0 = 1.0
Empirical formula	H_2O	

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Determine the empirical formula of a compound that contains 85.7% carbon and 14.3% hydrogen.

	Carbon (C)	Hydrogen (H)
Mass of each element (%)	85.7	14.3
Divide by atomic mass	85.7 / 12.0 = 7.142 mol	14.3 / 1.00 = 14.3 mol
Divide by lowest figure to get ratio	7.142 / 7.142 = 1.00	14.3 / 7.142 = 2.00
Empirical formula	CH_2	

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Molecular formula

- The molecular formula is the formula that shows the number and type of each atom in a molecule
- The molecular formula can be found by dividing the relative formula mass of the molecular formula by the relative formula mass of the empirical formula
- Multiply the number of each element present in the empirical formula by this number to

Question: The empirical formula of X is $C_4H_{10}S_1$ and the relative formula mass of X is 180. What is the molecular formula of X?

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Relative Formula Mass:
Carbon: 12
Hydrogen: 1
Sulfur: 32

Answer

- **Step 1:** Calculate relative formula mass of empirical formula

Relative formula mass = (C x 4) + (H x 10) + (S x 1)

Relative formula mass = (12 x 4) + (1 x 10) + (32 x 1)

Relative formula mass = 90

- **Step 2:** Divide relative formula mass of **X** by relative formula mass of empirical formula

Ratio between M_r of X and the M_r of the empirical formula = 180/90

Ratio between M_r of X and the M_r of the empirical formula = 2

- **Step 3:** Multiply each number of elements by 2

$(C_{4\times2}) + (H_{10\times2}) + (S_{1\times2}) = (C_8) + (H_{20}) + (S_2)$

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Molecular Formula of **X** is $C_8H_{20}S_2$

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4. Reacting masses and volumes (of solutions and gases)

4.1 Water of crystallisation

- Water of crystallisation is when some compounds can form crystals which have water as part of their structure
- A compound that contains water of crystallisation is called a **hydrated compound**
- The water of crystallisation is separated from the main formula by a dot when writing the chemical formula of hydrated compounds
  - Eg. hydrated copper (II) sulfate is $CuSO_4 \cdot 5H_2O$
- A compound which doesn't contain water of crystallisation is called an **anhydrous compound**
  - Eg. anhydrous copper (II) sulfate is $CuSO_4$
- A compound can be hydrated to different degrees
  - Eg. Cobalt (II) chloride can be hydrated by six or two water molecules
  - $CoCl_2 \cdot 6H_2O$ or $CoCl_2 \cdot 2H_2O$
- The conversion of anhydrous compounds to hydrated compounds is reversible by heating the hydrated salt
  - Anhydrous to hydrated salt (by adding water): $CuSO_4 + 5H_2O \rightarrow CuSO_4 \cdot 5H_2O$
  - Hydrated to anhydrous salt (by heating): $CuSO_4 \cdot 5H_2O \rightarrow CuSO_4 + 5H_2O$

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4.2 Reacting masses and volumes

$$\text{number of mol} = \frac{\text{mass of a substance in grams } (g)}{\text{molar mass } (g\ mol^{-1})}$$

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{predicted yield (theoretical yield)}} \times 100$$

$$\text{amount of gas (mol)} = \frac{\text{volume of gas } (dm^3)}{24}$$

$$\text{concentration (mol } dm^3) = \frac{\text{number of moles of solute (mol)}}{\text{volume of solution } (dm^3)}$$

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